Exact summation of vertex corrections to the penetration depth in d-wave superconductors

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A variety of experiments suggest that in the cuprates, the low-energy superconducting quasiparticles undergo forward scattering from extended impurity potentials. We argue that when such potentials dominate the scattering, the penetration depth may be computed in a simple zero-angle scattering approximation (ZSA), in which the vertex corrections to the Meissner effect may be summed exactly. We find a remarkably simple relationship between the normal fluid density and the quasiparticle density of states of the disordered system which holds for every realization of the disorder. We expect this result to be relevant to the *ab*-plane penetration depth in high-purity single crystals of underdoped YBCO.

PACS numbers: 74.25.Nf,74.72-h

Measurements of the in-plane penetration depth λ have been central to elucidating the nature of superconductivity in the high-temperature copper-oxide superconductors. Equally important has been the theoretical understanding of impurity scattering in d-wave superconductors required to interpret these measurements. The temperature dependence of $\lambda(T)$ provided the first strong evidence¹ for unconventional pairing symmetry. Subsequently, the effect on $\lambda(T)$ of isotropic elastic scattering from point-like in-plane impurities in a superconductor with $d_{x^2-y^2}$ pairing symmetry was investigated.² This picture of impurity scattering accounted for the observed crossover from a quadratic low-temperature behavior in $\lambda^{-2}(T)$ to the T-linear behavior at higher temperatures characteristic of a gap function with nodes.

More recently, it has been suggested in different experimental contexts that quasiparticles near the Fermi surface undergo forward scattering. Forward scattering from impurities has been invoked³ to account for a component of the single-particle scattering rate observed in angle-resolved photoemission (ARPES) spectra which apparently contributes negligibly to the normal state resistivity. Such scattering may arise from a smoothly varying in-plane potential due to the poorly screened⁴ Coulomb fields of disordered dopant oxygen ions residing between the CuO₂ layers. This potential may account for the nanoscale electronic inhomogeneity observed in scanning-tunneling spectroscopy (STS) studies of optimally to overdoped Bi₂Sr₂CaCu₂O_{8+x}.⁵ A flurry of recent activity^{6,7,8,9,10} is aimed in part at synthesizing the evidence for forward scattering in this compound obtained from ARPES, STS, and thermal and electrical conductivities.

At the same time, measurements of the microwave conductivity $\sigma(\omega, T)$ in YBCO present their own puzzles. High quality YBa₂Cu₃O_{6.993} crystals have shown a Drude-like phenomenology in the conductivity at low frequencies and temperatures.¹¹ In a nodal quasiparticle picture of low-energy charge transport¹², this implies significant frequency-independent part of the scattering rate, inconsistent with scattering by point defects. It has

been shown¹³ that extended linear defects such as twin boundary remnants can produce such behavior. However, precise bolometric measurements¹⁴ subsequently have shown deviations from Drude behavior at the lowest temperatures and frequencies as well as an unexpected $\omega/(T+T_0)$ scaling. Violation of the Wiedemann-Franz law and the universal conductivity limit¹⁵ in cuprates have also fueled theoretical interest in quasiparticle self-energy¹⁶ and transport^{17,18} in the presence of extended impurities.

Finally, extended disorder potentials have surfaced in a recent attempt¹⁹ to explain in a unified theory the doping and temperature dependence of both the c-axis and ab-plane penetration depth in underdoped YBCO. The theory models the incoherent interlayer hopping by scattering in-plane states by momenta of order Λ as they tunnel between the layers. Good agreement with recent c-axis data has been obtained²⁰ with $\hbar/\Lambda = 120$ Å, or about 25 lattice spacings. The effect of such interlayer disorder on in-plane transport is similar to that of inplane scattering potentials which extend over distances of order \hbar/Λ . Presumably, such potentials arise from the aforementioned disorder of interlayer oxygen dopants, which, unlike BSCCO, may dominate the scattering rate due to the very low cation disorder in high-purity YBCO crystals.

In this paper, we argue that the nodal structure of a d-wave superconductor presents an unusual situation in which even mildly extended potentials lead to strong forward scattering. The simplest approximation allowing for a sensible calculation of the superfluid density is the zero-angle scattering approximation (ZSA): the impurity potential is unable to modify upon scattering the charge current carried by a quasiparticle. Extended potentials induce elastic scattering by small momenta, implying that, except via rare internodal scattering events, nodal quasiparticles scatter exclusively within the same node. However, the quasiparticle velocity relevant to charge current varies much more slowly in the nodal region than does the energy, as it arises from the bare band-structure. The ZSA is thus expected to be valid when

extended potentials dominate the scattering rate. This is likely the situation in high-purity YBCO single crystals, in which smooth potentials due to interlayer dopants dominate the scattering.

The main result presented here is that under such circumstances the normal fluid density n_n is connected to the single-particle density of states per site per spin $\mathcal{N}(E)$ by the simple relation

$$\frac{n_n}{m^*} = \left(\frac{v_F}{a}\right)^2 \int dE \, \mathcal{N}(E)[-f'(E)],\tag{1}$$

where v_F is the magnitude of the quasiparticle velocity at the node and f is the Fermi-Dirac distribution. Since the electron density is the sum of the normal- and superfluid densities, this quantity dictates the temperature dependence of the penetration depth. It is remarkable that (1), which is a trivial result for the clean superconductor, continues to hold in the presence of extended disorder potentials, albeit with $\mathcal{N}(E)$ renormalized by the disorder. Since it is valid for every realization of the disorder, it circumvents the considerable complications of vertex corrections,¹⁷ which arise upon disorder-averaging twoparticle correlation functions. Furthermore, (1) does not require any particular model of the disorder (e.g. Born limit, ladder approximation,) though it reveals nothing about $\mathcal{N}(E)$ itself. Thus if the ZSA is valid, (1) is a powerful consequence allowing a model-independent interpretation of the normal fluid density.

The limitation of this approximation is that, as in the clean superconductor, the dissipative part of conductivity²⁴ $\sigma_1(\omega)$ becomes a δ -function at zero frequency. This is to be expected since zero-angle scattering cannot degrade the charge current. However, as in a clean superconductor at $T \neq 0$, a fraction of the superfluid is converted into normal fluid, which may be reliably computed despite the fact that the distribution of $\sigma_1(\omega)$ is unphysical. In the ZSA, this normal fluid behaves as a perfect metal, having infinite d.c. conductivity but making no contribution to the Meissner effect. In reality, small-angle (and rare internodal) scattering degrades this perfect metal and results in a dissipative conductivity peak of finite width. However, the ZSA can provide no information about the frequency distribution of $\sigma_1(\omega)$. We assume that such scattering is sufficiently weak that it primarily affects only the frequency distribution of $\sigma_1(\omega)$ and not the integral, so that Eq. (1) remains valid.

We consider the general Hamiltonian $H = H_K + H_{sc}$, with

$$H_{K} = \sum_{\mathbf{r},\sigma} \left[\frac{1}{2} (V_{\mathbf{r}} - \mu) c_{\mathbf{r},\sigma}^{\dagger} c_{\mathbf{r},\sigma} - t \left(c_{\mathbf{r}+\hat{\mathbf{x}}a,\sigma}^{\dagger} c_{\mathbf{r},\sigma} + c_{\mathbf{r}+\hat{\mathbf{y}}a,\sigma}^{\dagger} c_{\mathbf{r},\sigma} \right) - t_{\mathbf{r}}^{\perp} c_{\mathbf{r}+\hat{\mathbf{z}}d,\sigma}^{\dagger} c_{\mathbf{r},\sigma} \right] + \text{h.c.},$$

$$H_{sc} = \frac{1}{2} \sum_{\mathbf{r}} \left[\Delta_{\mathbf{r}+\hat{\mathbf{x}}a/2} \left(c_{\mathbf{r},\uparrow}^{\dagger} c_{\mathbf{r}+\hat{\mathbf{x}}a,\downarrow}^{\dagger} + c_{\mathbf{r}+\hat{\mathbf{x}}a,\uparrow}^{\dagger} c_{\mathbf{r},\downarrow}^{\dagger} \right) - \Delta_{\mathbf{r}+\hat{\mathbf{y}}a/2} \left(c_{\mathbf{r},\uparrow}^{\dagger} c_{\mathbf{r}+\hat{\mathbf{y}}a,\downarrow}^{\dagger} + c_{\mathbf{r}+\hat{\mathbf{y}}a,\uparrow}^{\dagger} c_{\mathbf{r},\downarrow}^{\dagger} \right) \right] + \text{h.c.}$$

$$(2)$$

It describes, at the mean-field level, a d-wave superconductor on square-lattice layers with in-plane lattice constant a and interlayer spacing d. The interlayer hopping $t^{\perp}_{\mathbf{r}}$ (which may model the incoherent c-axis transport as in Ref. 19) and the on-site potential $V_{\mathbf{r}}$ are assumed to be weak relative to t and have a zero average value. The order parameter $\Delta_{\mathbf{r}}$ is defined on lattice bonds and may also vary weakly (compared to its average value) due to the disorder potentials. These quantities are assumed to vary slowly along the in-plane directions over the length scale \hbar/Λ but may vary randomly from layer to layer.

It will be convenient to work with the Nambu spinor $\Psi_{\mathbf{r}} \equiv (c_{\mathbf{r},\uparrow},c_{\mathbf{r},\downarrow}^{\dagger})^T$. The Hamiltonian (2) may be diagonalized by a Bogliubov transformation to $H = E_0 + \sum_{n,\sigma} \epsilon_n \gamma_{n,\sigma}^{\dagger} \gamma_{n,\sigma}$ where E_0 is the ground state energy and ϵ_n labels the (positive) quasiparticle excitation energies. The γ operators obey the usual fermion commutation relations up to a renormalization constant: $\{\gamma_{\mathbf{r},\sigma},\gamma_{\mathbf{r}',\sigma'}^{\dagger}\}=N\delta_{\mathbf{r},\mathbf{r}'}\delta_{\sigma,\sigma'}$ where N in a finite system is the number of lattice sites. The transformation can be compactly represented using a two-component wave-

function $\mathfrak{u}^{(n)}(\mathbf{r}) = (u_n(\mathbf{r}), v_n(\mathbf{r}))^T$. Introducing the antisymmetric tensor ε , we write (with the sums over tensor indices implicit hereafter,) $\gamma_{n,\uparrow}^{\dagger} = \sum_{\mathbf{r}} (\Psi_{\mathbf{r}}^{\dagger})_{\alpha} \mathfrak{u}_{\alpha}^{(n)}(\mathbf{r})$ and $\gamma_{n,\downarrow} = \sum_{\mathbf{r}} \varepsilon_{\alpha\alpha'}(\Psi_{\mathbf{r}}^{\dagger})_{\alpha'} \mathfrak{u}_{\alpha}^{(n)*}(\mathbf{r})$. The wavefunctions satisfy the orthogonality relations

$$\frac{1}{N} \sum_{\mathbf{r}} \mathfrak{u}_{\alpha}^{(n)}(\mathbf{r}) \mathfrak{u}_{\alpha}^{(n')*}(\mathbf{r}) = \delta_{n,n'},$$

$$\frac{1}{N} \sum_{\mathbf{r}} \varepsilon_{\alpha\beta} \mathfrak{u}_{\alpha}^{(n)}(\mathbf{r}) \mathfrak{u}_{\beta}^{(n')}(\mathbf{r}) = 0.$$
(3)

With this notation, the in-plane components of current are $\mathcal{J}_{x(y)}(\mathbf{r}) \equiv it(\Psi_{\mathbf{r}+\hat{\mathbf{x}}(\hat{\mathbf{y}})a}^{\dagger}\Psi_{\mathbf{r}} - \Psi_{\mathbf{r}}^{\dagger}\Psi_{\mathbf{r}+\hat{\mathbf{x}}(\hat{\mathbf{y}})a})$. In the disordered system, $n_n/m^* = \Pi_{xx}(0)$ where the long-wavelength polarization function is $\Pi_{\mu\nu}(i\omega) \equiv \frac{1}{N}\sum_{\mathbf{r},\mathbf{r}'}\int_0^\beta d\tau\,e^{i\omega\tau}\,\langle\mathcal{T}_\tau\mathcal{J}_\mu(\mathbf{r},\tau)\,\mathcal{J}_\nu(\mathbf{r}',0)\rangle$. It is also useful to introduce a vertex function which describes the coupling of long-wavelength radiation to electrons at lattice sites \mathbf{r}_1 and \mathbf{r}_2 ,

$$\lambda_{x(y)}(\mathbf{r}_1, \mathbf{r}_2) \equiv it(\delta_{\mathbf{r}_1, \mathbf{r}_2 + \hat{\mathbf{x}}(\hat{\mathbf{y}})a} - \delta_{\mathbf{r}_2, \mathbf{r}_1 + \hat{\mathbf{x}}(\hat{\mathbf{y}})a}). \tag{4}$$

Importantly, the Hamiltonian (2) describes a non-interacting system, and we may apply Wick's theorem to evaluate Π . We assume that $\langle \mathcal{J} \rangle = 0$ in the unperturbed system, in which case Π may be expressed

$$\Pi_{xx}(i\omega) = -\frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}_2} \sum_{\mathbf{r}_1', \mathbf{r}_2'} \lambda_x(\mathbf{r}_1, \mathbf{r}_2) \lambda_x(\mathbf{r}_1', \mathbf{r}_2')$$

$$T \sum_{i\nu} \text{Tr} \left[G(\mathbf{r}_2, \mathbf{r}_1'; i\nu + i\omega) G(\mathbf{r}_2', \mathbf{r}_1; i\nu) \right] \tag{5}$$

in terms of the matrix Green function $G(\mathbf{r}, \mathbf{r}'; i\nu) \equiv -\int_0^\beta d\tau \ e^{i\nu\tau} < \mathcal{T}_\tau \Psi_{\mathbf{r}}(\tau) \Psi_{\mathbf{r}'}^{\dagger}(0)>$. We will make use of the spectral function $A(\mathbf{r}, \mathbf{r}'; \omega) \equiv (2\pi i)^{-1} [G^A(\mathbf{r}, \mathbf{r}'; \omega) - G^R(\mathbf{r}, \mathbf{r}'; \omega)]$ which has the representation

$$A(\mathbf{r}, \mathbf{r}'; \omega)_{\alpha\beta} = \frac{1}{N} \sum_{n} \left[\delta(\omega - \epsilon_{n}) \mathfrak{u}_{\beta}^{(n)}(\mathbf{r}) \mathfrak{u}_{\alpha}^{(n)*}(\mathbf{r}') + \delta(\omega + \epsilon_{n}) \varepsilon_{\alpha\alpha'} \varepsilon_{\beta\beta'} \mathfrak{u}_{\alpha'}^{(n)}(\mathbf{r}') \mathfrak{u}_{\beta'}^{(n)*}(\mathbf{r}) \right].$$

$$(6)$$

We now state the ZSA precisely, establish its validity, and derive (1). We define

$$Q_x(\mathbf{r}_1, \mathbf{r}_2; \omega) \equiv \sum_{\mathbf{r}'} \lambda_x(\mathbf{r}_1, \mathbf{r}') A(\mathbf{r}', \mathbf{r}'_2; \omega), \tag{7}$$

whose trace and integral over ω gives $2\lambda_x$. The quantity Q_x may be regarded as a decomposition of λ_x in terms of quasiparticle energies ω . Eq. (5) for the polarization becomes

$$\Pi_{xx}(i\omega) = -\frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}_2} \int dE \, dE' \, \frac{f(E) - f(E')}{i\omega - (E' - E)} \tag{8}$$

$$\operatorname{Tr} \left[Q_x(\mathbf{r}_1, \mathbf{r}_2; E) Q_x(\mathbf{r}_2, \mathbf{r}_1; E') \right].$$

The ZSA is implemented in the disordered system by approximating Q_x by a form which is valid for low-lying quasiparticle energies E, E'.

To find such an approximation, it is instructive to view $\lambda_x(\mathbf{r}_1, \mathbf{r}_2)$ as the kernel of an integral operator, which we call the "vertex operator". To illustrate, we rewrite (4)

$$\lambda_x(\mathbf{r}_1, \mathbf{r}_2) = \iint \frac{d^2(ka)}{(2\pi)^2} 2t \sin(k_x a) e^{i\mathbf{k}\cdot\mathbf{r}_1} \left(e^{i\mathbf{k}\cdot\mathbf{r}_2}\right)^*. \tag{9}$$

The vertex operator thus has eigenvalues $2t\sin(k_x a)$ and plane-wave eigenvectors. On the other hand, the quasiparticle wavefunctions of the *clean* system (i.e. $V_{\bf r}=0$, $t_{\bf r}^\perp=0$, and $\Delta_{\bf r}$ constant) are also plane waves. The δ -function behavior of conductivity in the clean system arises precisely because the vertex function and the Hamiltonian are diagonal in the same basis, i.e. the vertex operator commutes with H. In the disordered system, H is diagonalized by the wavefunctions $\mathfrak{u}^{(n)}$ and thus does not commute with the vertex operator, making $\sigma_1(\omega)$ regular.

A low-energy effective vertex operator for the clean system is obtained by restricting \mathbf{k} in (9) to the vicinity

of a node \mathbf{q} . Under this restriction, the eigenvalue is weakly \mathbf{k} -dependent. Thus we make the approximation

$$2t\sin(k_x a) \to \pm v_F/a\sqrt{2},\tag{10}$$

the sign depending on the node. The leading k-dependent term $(k_x - q_x)/m^*a$ leads in the clean system to a correction to (1) whose relative size we estimate as $(2\eta T/m^*v_F^2)^2$ where $\eta > 1$ is the anisotropy of the linearized nodal dispersion. For the particular bandstructure of (2), $m^*v_F^2 = 4t \sin q_x a \tan q_x a$, which is nominally of order 4t but diverges rapidly as half-filling is approached. Furthermore, $\eta T_c \ll 4t$ in underdoped cuprates, making (10) an excellent approximation.

The approximate vertex operator arising from (10) is, within the subspace of a single nodal region, simply a constant multiple of the identity operator. This powerful simplification may be applied to the disordered system given two assumptions. We first assume that the lowenergy wavefunctions in the disordered system are linear combinations of low-energy wavefunctions in the clean system. We thus neglect the contribution of low-energy states which may arise from the mixing of anti-nodal states. 16 Since the anti-nodes are connected by wavevectors of order a^{-1} , such low-energy states should constitute a negligible portion of the spectral density when $\Lambda a \ll 1$. Second, we assume that the extended impurities produce negligible internodal scattering. Degenerate plane-wave states from different nodes will hybridize and split by an energy of order |V'|, where V' is a typical matrix element for scattering between nodes. Assuming the Fourier spectrum of $V_{\mathbf{r}}$ to be exponential with width Λ , we estimate $|V'| \sim V_0 e^{-|\delta q|/\Lambda}$ where δq is the relative momentum between nodes and V_0 is the RMS value of the potential $V_{\bf r}$.²⁵ Already $|V'| \ll V_0$ when Λ^{-1} is comparable to just a few lattice spacings. We assume that relevant experiments are in the regime $T \gg |V'|$, so that these hybridized states are essentially degenerate.²⁶ We may then choose a basis for the low-energy sector of the disordered system in which each state resides near a single node.

Thus, in the regime $|V'| \ll T \ll 4t/\eta$, it becomes trivial to express the vertex operator in the quasiparticle basis of the disordered system. We denote the eigenvalues as $\lambda_x^{(n)} = \pm v_F/a\sqrt{2}$, the sign depending on the node of state n. Then (7) becomes

$$Q_{x} \to \frac{1}{N} \sum_{n} \lambda_{x}^{(n)} \left[\delta(\omega - \epsilon_{n}) \mathfrak{u}_{\beta}^{(n)}(\mathbf{r}_{1}) \mathfrak{u}_{\alpha}^{(n)*}(\mathbf{r}_{2}) - \delta(\omega + \epsilon_{n}) \varepsilon_{\alpha\alpha'} \varepsilon_{\beta\beta'} \mathfrak{u}_{\alpha'}^{(n)}(\mathbf{r}_{2}) \mathfrak{u}_{\beta'}^{(n)*}(\mathbf{r}_{1}) \right],$$

$$(11)$$

which may be regarded as the precise statement of the ZSA. Since the time reversal transformation on wavefunctions is $\mathfrak{u}_{\alpha}^{(n)}(\mathbf{r}) \to \varepsilon_{\alpha\alpha'}\mathfrak{u}_{\alpha'}^{(n)*}(\mathbf{r})$, the second term in (11) corresponds to the time-reversal of the first and acquires a sign change. The orthogonality relations (3) allow us

to evaluate

$$\frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}_2} \operatorname{Tr} \left[Q_x(\mathbf{r}_1, \mathbf{r}_2; E) Q_x(\mathbf{r}_2, \mathbf{r}_1; E') \right] =$$

$$\frac{1}{2} \left(\frac{v_F}{a} \right)^2 \delta(E - E') \frac{1}{N} \sum_{\mathbf{r}} \left[\delta(E - \epsilon_n) + \delta(E + \epsilon_n) \right].$$
(12)

Substituting into (8) leads directly to main result (1), with the density of states per site per spin \mathcal{N} given by

$$\mathcal{N}(\omega) \equiv \frac{1}{2N} \sum_{n} [\delta(\omega - \epsilon_n) + \delta(\omega + \epsilon_n)]. \tag{13}$$

We note that (1) can also be obtained²¹ using the diagram method²² for disorder-averaged correlation functions. In this context, zero-angle scattering at the nodes allows vertex correction diagrams to be summed exactly and expressed in terms of the single-particle Green function. This simplification is formally analogous to the diagrammatic Ward-Takahashi identity²³ of quantum electrodynamics, by which the longitudinal component of the interacting vertex function may be expressed in terms of the interacting Green function. In our context, however, (1) has nothing to do with electromagnetic gauge invariance, but arises instead from the fact that i) the Hamiltonian (2) is noninteracting and ii) the effective vertex function for the low-energy states has trivial structure, as we have argued above.

In ordinary metals forward scattering leads to a reduction of the transport scattering rate $1/\tau_{\rm tr}$ compared to the single-article scattering rate $1/\tau$. The result presented above can be viewed as an extreme example of

this effect in a system of nodal fermions where $1/\tau$ is finite but $1/\tau_{\rm tr}$ is reduced essentially to zero. This illustrates the singular nature of the vertex corrections that have been summed to obtain (1). It is also interesting to note that the superfluid density, ordinarily considered a transport quantity, depends only on the single-particle scattering rate in this case.

We have derived the remarkably simple result (1), which relates the normal fluid density to the quasiparticle density of states in a system disordered with extended impurities. The normal fluid density may be computed in the ZSA in spite of the fact that, as in a clean superconductor, the real part of conductivity becomes a δ -function at zero frequency. This derivation proceeds directly from the quasiparticle wavefunctions $\mathfrak{u}^{(n)}$ and energies ϵ_n of Hamiltonian (2), showing that (1) holds for individual realizations of the disorder and thus circumvents the considerable complications of vertex corrections. It therefore allows for a model-independent inversion of $n_n(T)$ from experiment to obtain the density of states. To theoretically predict $\mathcal{N}(E)$ and $\sigma_1(\omega)$, however, requires a more specific, model-dependent calculation. Eq. (1) may be applicable to high-purity single crystals of underdoped YBCO, in which slowly varying potentials from interlayer dopant disorder dominate the low energy scattering.

We acknowledge A. J. Berlinsky, D. A. Bonn, T. P. Davis, C. Kallin, and M. Schechter for helpful discussions. This work was supported by NSERC, CIAR, and the A. P. Sloan Foundation. The authors are indebted to Aspen Center for Physics where this work was initiated.

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Hereafter we use $\sigma_1(\omega)$ and "conductivity" to denote only the normal fluid component.

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²⁶ Beyond the ZSA, the splitting of these states governs the broadening of the δ -function in conductivity.